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LETTER FROM THE PRESIDENT

Letter from the President



Henk Schenk

In this letter I will inform you about the change of venue of the IUCr General Assembly and Congress 2002 from Jerusalem to Geneva.

The organisation required for a Congress as large as ours means that it is not easy to change to another venue at the last minute. Indeed, a lead time of more than a year is essential. Therefore, over the winter the Executive Committee and the Organising Committee have been discussing the present situation in the Middle East in relation to the 2002 IUCr General Assembly and Congress, scheduled to be held in Jerusalem. We concluded that with the present coverage of events in the area many potential participants would be reluctant to participate. Also the business of the IUCr would be affected as Commissions should meet, the General Assembly should discuss the next triennium, the Executive Committee should meet, etc. We decided that we had to move the meeting to an alternative venue in the event that no significant progress was made to improve the existing situation in Israel.

When we started the discussion about the situation with Joel Bernstein, the chair of the local Organising Committee, it was clear that our Israeli colleagues were all fully committed to organising an outstanding meeting in every way. Indeed, they even were already anticipating that an unfavourable situation might arise and that it would not be possible to organise the Congress in Jerusalem. When we later started to discuss a possible new venue we were also very happy to find the full understanding and support of our Swiss colleagues.

To our deep regret nothing significant had happened to improve the situation by the end of March. Therefore we have taken the decision to change the venue. We are well aware that this is very sad for our Israeli colleagues and feel very sorry for them as they were looking forward to acting as our host in Israel in 2002. However, as a vital and non-political organisation we have to move forward and cannot afford to lose momentum by having a partial General Assembly and Congress or, indeed, none at all.

We are happy that our Israeli colleagues are still enthusiastically involved in the organisation as can be seen from the following statements summarising the results of the discussions:

1. The new venue will be Geneva, Switzerland, in the Palexpo Congress Centre.
2. The 2002 General Assembly and Congress remains the 'Israeli' Congress, organised in another country by the agreed Committees.
3. The Swiss National Committee for Crystallography agrees on the venue and offers help to the Organising Committee.

I wish to thank all the individuals involved in the extensive discussions and their support for the change.

We in the Executive Committee are convinced that our Israeli colleagues will organise an excellent 2002 General Assembly and Congress in this new setting and look forward to seeing you all from 6 to 15 August 2002 in Geneva.

Henk Schenk
schenk@chem.uva.nl

EDITORIAL

Editorial



The cover story in this issue of the *IUCr Newsletter* concerns the remarkable new improved Protein Data Bank (PDB). The PDB holds the key to determining the functions of the tens of thousands of protein products of the human, plant, animal, and bacterial genomes that are being sequenced with ever increasing rapidity. Most estimates suggest that the functions of 250,000 genes in the SWISS-PROT and TrEMBL Database are unknown. If the scientific community is going to meet the challenge of determining the functions of these hypothetical proteins and uncover the structural details required to make it possible to control and use the proteins for the benefit of mankind, the PDB may well be the most important scientific resource in the world. The new PDB has a remarkable range of activities that go well beyond the gathering and distribution of protein and nucleic acid crystal structure data. Those activities are outlined in the annual report for 2000 from which the report on page 25 was drawn. The cover illustration reflects the increase in number and size of protein structures being deposited in the database each year since it began.

This issue of the newsletter also includes two announcements of recent developments that are very important to the world community of crystallography, the merge of two major manufacturers of X-ray diffraction equipment, Bruker AXS and Nonius (page 20) and the change of venue of the 19th Congress and General Assembly of the IUCr, July 6-15, 2002 from Jerusalem to Geneva, Switzerland. The next issue of the newsletter will contain additional information about the meeting site in Geneva.

It saddens me to report the recent deaths of three leaders in the crystallographic community, G.N. Ramachandran, winner of the 1999 Ewald Prize, M.A. Viswamitra of the Physics Dept, Indian U. of Science, Bangalore, and Jan Kroon, Head of the Dept of Crystal and Structural Chemistry, U. Utrecht in the Netherlands.

As the IUCr newsletter begins its ninth year, I want to express my continued appreciation to the advertisers without whose support the newsletter could not be provided to the international crystallographic community. I also want to thank all those who have contributed news items, meeting reports, and announcements of future activities in their countries.

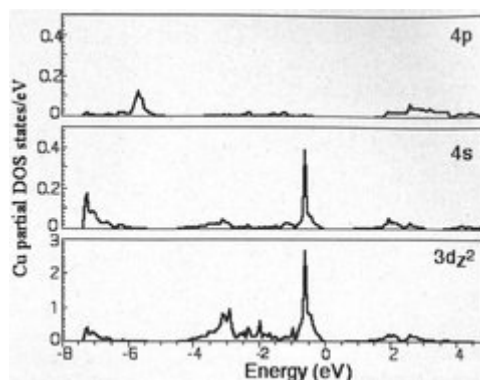
Four issues of the IUCr Newsletter were printed in 2000. The content covered IUCr activities, regional affiliates, news concerning crystallographers and crystallography, notices, awards, and elections, resources, obituaries, meeting reports, future meeting announcements, and a general calendar. Each issue contained 32 pages, a 33% increase over the previous year's content. The amount of material contributed from different countries especially Japan, India, and Africa, grew significantly.

Please send contributions concerning crystallography in your country, so that the newsletter can continue to reflect the unity of a community that recognizes no political boundaries.

Bill Duax
(duax@hwi.buffalo.edu)

LETTER TO THE EDITOR

Letter to the editor



LAPW partial density of states at Cu in cuprite. Peaks indicate hybridization of $3d_{z^2}$ partially unoccupied and holes in the experimental difference map. There's no evidence of hybridization of $4p$, suggested by Wang and Schwartz (*Angew Chem. Int Ed* 2000, **39**, 21)

Dear Bill,

An exchange of letters between Spackman *et al.*, Humphreys and Coppens (*IUCr Newsletter*, Vol. 8, Nos 1 and 3), commenting on our combined electron and X-ray diffraction measurement of charge-density in cuprite (*Nature*, **401**, p. 49, 1999), raised three substantial points.

1. *Accuracy of methods*. Is kinematic X-ray diffraction sufficiently accurate to give meaningful charge densities? What standard is meaningful? If our goal is to understand bonding, we must compare experiment and theory. Due to recent progress, charge densities can be calculated with an accuracy comparable to the best experimental measurement [e.g. Pendellösung X-ray, Convergent-Beam Electron Diffraction (QCBED) data]. For the silicon standard, experiment and local density approximation (LDA) theory agree to within 0.24% (*R* factor), while LDA differs from Generalised Gradient Approximation theory by 0.1% (*J. Phys.* **C9**, 7541, 1997). The accuracy of kinematic X-ray work is limited by extinction. A detailed comparison of electron and X-ray data revealed that the error in the X-ray data, corrected for extinction, is about 1%, twice the structure factor difference between superimposed ions and the crystal for the three lowest order structure factors (*Angew. Chem. Int. Ed.* 2000, **39**, p. 3791). We believe that this situation is typical for most inorganic materials referred to by Spackman, since the difference between results reported by different groups using different samples of the same material usually exceed experimental errors. The uncorrectable errors are due to statistical variation in the mosaic block distribution, and differences in crystal samples. QCBED patterns are taken from volumes of the order of 10^4 nm^3 , much smaller than one 'mosaic block', allowing use of the many-beam perfect crystal theory. Electron diffraction also benefits from the fact that electron intensities increase inversely as the scattering angle to the fourth power for the low angle bond-sensitive reflections. Our results for low order in MgO (*P.R. L.* **78**, p. 4777, 1998), NiO (*Phys. Rev.* **B61**, p. 2506, 2000) and cuprite are the most accurate, lie closest to *ab-initio* band-structure calculations, and, with the Pendellösung results, are indeed the only ones capable of distinguishing many-electron approximations in the theory. The MgO work achieved a tenfold improvement in accuracy over previous X-ray work. The critical voltage method (Smart and Humphreys *Inst. Phys. Conf. Ser.* **52**, p. 211, 1980) provides comparably accurate ratios of structure factors. Three-phase invariants may be measured by many-beam electron diffraction with better than one degree accuracy in phase (*Acta Cryst.* **A49**, 422, 1993), *P.R.L.* **62**, 547, 1989).

2. *Use of the term 'orbital'*. We agree with Scerri (*J. Chem. Ed.* **77**, p. 1492, 2000) that orbital wavefunctions are unobservable and that 'the orbital model remains enormously useful...and lies at the heart of much of computational chemistry; but it is just that, a model'. Aware of this, we use many-electron theory in all the calculations reported in our paper. However, it would be perverse not to mention the resemblance of the shape of the hole in our difference map to the simple one-electron

model of a d -orbital charge-density distribution. This similarity indicates that the one-electron model retains validity, even in a transition metal oxide, and that one particular choice of basis functions converges more efficiently than others. Continued use of terms and concepts such as 'd-electron', 'molecular orbital diagram', 'orbital degeneracy', 'orbital angular momentum', 'anti-bonding orbital' etc. by workers in the field suggests that one-electron theory is too useful an approximation to be abandoned.

3. *The significance of difference charge density.* Our charge density image shows the difference between the experiments and the spherical ion model of Cu^+ and O^{2-} . the negative difference charge density around Cu is due to the d_z^2 hole formed by $3d_z^2$ and $4s$ hybridization, a picture supported by both theory and experiment (Marksteiner *et al.*, *Zeit. Phys.* **B64**, 119 (1989); Grioni *et al.*, *Phys. Rev.* **B45**, 3309 (1992)). The figure above shows the partial density of states around Cu calculated by the LAPW method. Restori and Schwarzenbach, (*Acta Cryst.* **B42**, 201, (1986)) show that in the molecular-orbital model the charge density around Cu is a sum of partially occupied $|\psi_z^2|^2$ and $|\psi|^2$, other fully-occupied d -states and the interference terms, $\text{Re}(\psi_z^2 \psi_s)$ and $\text{Re}(\psi_{xz} \psi_{yz})$. These, when subtracted from the charge density of a closed-shell Cu^+ with a fully occupied d_z^2 state, would give a negative charge density for $|\psi_z^2|^2$. The resemblance of our difference map to the d_z^2 orbital arises from the fact that the radial distributions are very different for the d_z^2 (<1) and $4s$ (>1) electrons, thus spatially separating the d_z^2 and $4s$ electrons. The agreement between this single-electron model and our experiment, supported by many-electron calculations and spectroscopic evidence, vindicates the quantum mechanical single electron approximation for this case.

In closing, we note that while the electron community has consistently taken full account of X-ray works (which is vital, since QCBED remains inaccurate for high orders and temperature factors), this practice has rarely been reciprocated. It seems clear that both methods are needed for greatest accuracy, especially for high symmetry inorganic materials with small unit cells.

J.C.H. Spence, J.M. Zuo* and M. O'Keefe ASU (spence@asu.edu)

*UIUC (jianzuo@uiuc.edu)

LETTER TO THE EDITOR

Letter to the Editor

Dear Bill,

As one who did his first Fourier summations (2-D, and 3-D Harker sections) with Beevers-Lipson strips (incidentally, one can do structure-factor calculations with them, too), I would like to say that the process was not actually 'unthinkable' - the alternative then was log tables! They remain a useful teaching device for what is actually going on in a Fourier summation. I agree with Bob Gould (page 25 of Vol. 8 No. 3, 2000) about the mental arithmetic - it was faster than the calculators available at that time. I am pleased to have preserved the memory, at least, of Beevers-Lipson strips in a book, with my colleague R.A. Palmer, on Structure Determination by X-ray Crystallography (Chapter 6) - 4th Edition appearing later this year.

Mark Ladd (m.ladd@surrey.ac.uk)

LETTER TO THE EDITOR

Letter to the Editor

Bill,

Just a line of congratulations on a very good issue of the *IUCr Newsletter* (Vol 8, No 4). I have in mind, for example, the breast cancer diagnosis article on p.8 and the hydrogen-bond meeting report on p.19, to say nothing of the good stuff on Crystallography Journals Online and CIF developments, etc.

Of course I realise that you must be rather in the hands of the contributors when it comes to content, so maybe in part we're all just fortunate that a number of items of high general interest came together this month.

Robin Shirley (R.Shirley@surrey.ac.uk)

Dear Robin,

Thank you for your comments and thanks to all those who are contributing the material that gives this newsletter value and brings our international community together.

Bill

LETTER TO THE EDITOR

Letter to the Editor

Dear Editor

I am a master student at U. Teknologi Malaysia, Malaysia.

I've tried several times to get the SiGe alloys XRD standard data and it's not available here in our country. Can someone please help me regarding this semiconductor materials?

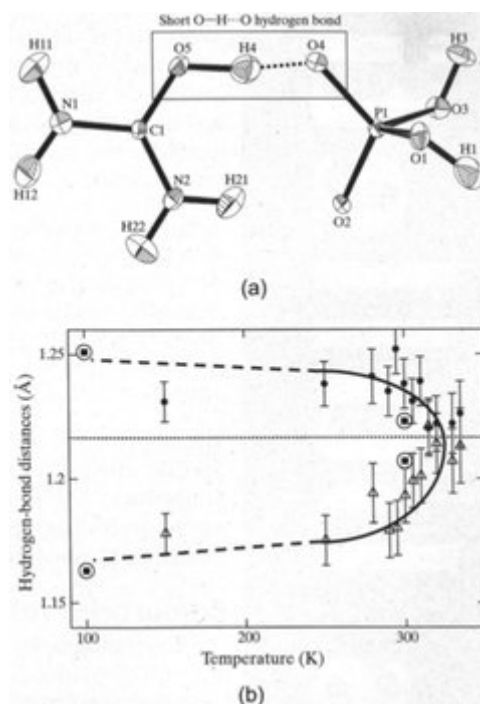
I really need this information for my research.

Thank You!

Suriati Bte Paiman (p.suria@rocketmail.com)

Migration of the proton in the strong O-H...O hydrogen bond in urea-phosphoric acid (1/1)

Chick C. Wilson, *Acta Cryst.* (2001). B57, 435-439



(a) ORTEP (Johnson, 1971) plot of the urea-phosphoric acid structure at 150 K, showing the atomic numbering and the strong O-H...O hydrogen bond. Note that partial transfer of the H atom (elongation of O5-H4) is indicative of significant formation of the salt uronium phosphate. Probability ellipsoids are drawn at the 50% level. (b) The increasingly symmetric location of the proton in the short, strong hydrogen bond in urea-phosphoric acid is illustrated by the convergence of the 'bonded' (O5-H4; open triangles) and non-bonded (H4...O4; filled circles) distances as the temperature increases. Also shown on this plot (as filled squares inside circles— error bars omitted for clarity) are the values found by Harkema at 100 K (unpublished work) and by Kostansek & Busing (1972) at room to the eye and the dotted line indicates the 'centred' situation found here above ~300 K.

The author reports a fascinating new result in a very topical area of structural chemistry and additionally a new method of recording time-of-flight Laue neutron diffraction data at ISIS (Chilton, Didcot, UK) from 'multiple' single crystals. The paper shows the temperature-dependent movement (~ 0.035 Å) of the proton in a short O-H...O hydrogen bond in the co-crystal of urea and phosphoric acid and an effectively symmetrical disposition at the highest temperature studied. Diffraction data were recorded at 14 temperatures between 150 and 335 K in steps of 5, 10 and 50 K and very useful experimental details are given in the text. The results are of general interest because of implications concerning the shape of the hydrogen-bond potential.

The author is an expert in single-crystal neutron diffraction using time-of-flight techniques and has developed a method for using multiple samples of molecular crystals. This can lead to a reduction in data collection times by the use of several rather smaller, deliberately misaligned crystals, mounted together in the cryorefrigerator. Previous experiments attempted in this area are reviewed and compared with this latest method used on the SXD single-crystal machine at ISIS, which was developed primarily for examining H-atom parameters in a variety of molecular crystals. The title compound provides an

example of a rather short O-H...O interaction, whose complex nature cannot be described from X-ray data alone, namely whether there's a complete or partial proton transfer to form a salt or whether the H atom remains localized as in a simple adduct.

The relatively low data-to-parameter ratios in the GSAS refinements (Larson & Von Dreele, 1994) are justified by the successful outcomes reported, i.e., the normal appearance of anisotropic displacement parameters and the acceptable standard uncertainties of the atomic coordinates. The model from a previous, conventional neutron diffraction study at 150 K was used as the overall starting point and each new refinement at one temperature was used as the starting model for refinement at each subsequent temperature. The geometry of the hydrogen bond is very clearly temperature dependent in this short O-H...O interaction, showing that the proton migrates towards the centre of the O...O separation at the higher temperature (see figure). By contrast, two other O-H...O 'normal' intermolecular hydrogen bonds in the crystal structure show no such marked H-atom migrations, just a slight increase in the H...O *non*-bonded separation over the same temperature range and both values are significantly longer than those under discussion here (1.5-1.7 Å *cf.* 1.18-1.25 Å).

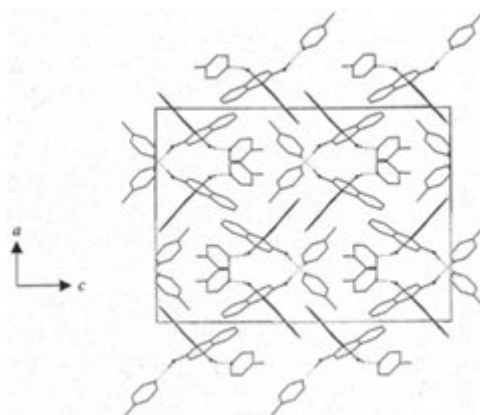
Reviewed by Judith A.K. Howard, Chemistry Dept, U. of Durham, UK

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Inclusion compounds of binaphthol with picolines: structures, selectivity and kinetics of desolvation

Luigi R. Nassimbeni & Hong Su, *Acta Cryst.* (2001). B57, 394-398



Projection along [010] for BNP4P. The hydrogen bonding is shown as dotted lines. The O atoms on the host are shown as solid balls and the N atoms on the guest as grey balls. All H atoms except the hydroxyl H atoms on the host are omitted.

The authors present some interesting work in the field of molecular recognition through this study of host-guest systems for which they have determined the crystal structures and thence their lattice energies. The results of further experiments allow correlation of the structures to thermal stability, energy of enclathration and the kinetics of desolvation. The choice of this bulky and rigid host, 2,2'-dihydroxy-1,1'-binaphthyl (binaphthol, BNP) follows earlier work by these authors and others and of particular interest are those systems where chiral guests have been embedded in the resolved host molecules.

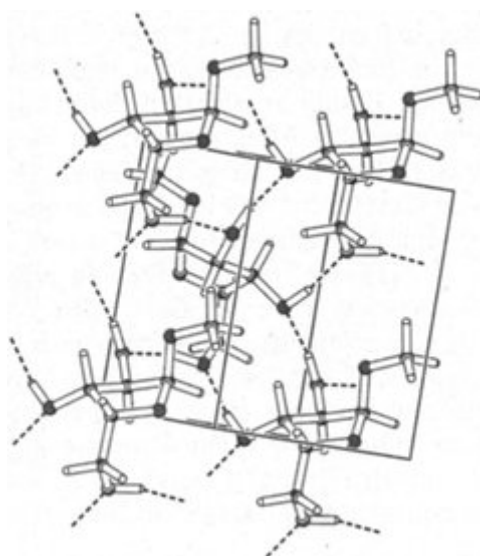
The structures of the three inclusion compounds were determined from low-temperature, single-crystal X-ray data (CCD) and all show some disorder in the methyl groups of the guest molecules. The three isomers of picoline, 2-, 3- and 4-methylpyridine (2P, 3P and 4P, respectively), were selected as guest molecules and these co-crystallize with binaphthol in different space groups, $C2/c$, $P2_1/c$ and $Pbca$. Each guest molecule relates through the picoline N atom to its host hydroxyl groups by O-H...N hydrogen bonds varying between 2.697 and 2.779 Å. The cross-sectional areas of the channels in the structures in which the guest molecules are located are calculated as 5.5×5.5 , 5×6 and 7×8 Å² and the change in conformation of the host molecules is marked by the increase in torsion angle about the C-C bond linking the two halves of the binaphthyl group, from 83.5, to 95.3 to 103.0° for the three picoline isomers, respectively.

The thermodynamic data presented in the paper suggest that 2- and 4-picoline are preferentially enclathrated over 3-picoline, which correlates with their calculated lattice energies in the order $4 > 2 > 3$. The difference between the energies calculated for 2- and 4-picoline, however, is small (3.2 kJ mol⁻¹) and this in turn fits with the observation of concentration dependence for the competition experiments for all three isomers, suggesting kinetic effects are also involved. TGA and DSC results on the compounds support these data, indicate a one-step desolvation and confirm the host-guest ratio of 1:2 observed in the crystal structures. The paper is well illustrated and referenced to other clathrate systems and the methodology used for the various thermodynamic calculations.

Reviewed by Judith A.K. Howard, Chemistry Dept, U. of Durham, UK

Structures of furanosides: geometrical analysis of low-temperature X-ray and neutron crystal structures of five crystalline methyl pentofuranosides

Artem Evdokimov, A. Joseph Gilboa, Thomas F. Koetzle, Wim T. Klooster, Arthur J. Schultz, Sax A. Mason, Alberto Albinati & Felix Frolow, *Acta Cryst.* (2001). B57, 213-220



Methyl α-D-xylofuranoside crystal packing diagram.

The paper reports an interesting study of five methyl pentofuranosides by low-temperature crystallography, whereby the crucial role of hydrogen bonding in this series can be discussed in detail for the first time, together with the wide-ranging conformations observed for the five-membered rings using accurate neutron diffraction results. The important context of the furanoside structures is reviewed with significant references to the literature, and the relevance of highly accurate crystal structures to modern modelling approaches in these compounds is discussed. Hitherto, data for only two methyl furanoside structures had been reported in the literature, so this paper represents a most important addition to the databases.

Previously in 1983, Jeffrey & Mitra had developed a method for classifying the hydrogen-bonding patterns observed in the then known crystal structures of 58 pyranoses and pyranosides and one furanoside into four types, and with the exception of methyl β-D-ribofuranoside, these new compounds all fall into classes I or III. Herein, however, the authors opted to use the Marzec & Day (1993) system of describing the exact geometry of the five-membered rings, using five bond lengths and four conformational variables, based largely on the Cremer & Pople (1975) descriptors, namely the pseudo-rotation angle ($\mathbf{P}$, °), the maximum deviation along the normal to the Cremer-Pople plane ($\mathbf{q}$, Å), the distortion of the ring in the Cremer-Pople plane ($\mathbf{s}$, Å) and the direction of $\mathbf{s}$ (Γ , °). The authors compare and analyse these nine derived parameters of the methyl furanosides with one another and with the related methyl hexopyranosides, which naturally show less ring strain and any subsequent effects upon the ring geometry. The bond lengths for both series are remarkably similar, while bond angles are consistently smaller for the furanosides (4-8°). The extensive hydrogen-bonding network is entirely *intermolecular* in these crystal structures. The ring conformations show a wide range of pseudo-rotational phase angles, with a more closely averaged cluster of $\mathbf{q}$, $\mathbf{s}$, and Γ values. The authors discuss

the differences and similarities in these conformations with those from several hundreds of known ribo- and deoxyribofuranoside rings in DNA, RNA and nucleosides/tides, bearing in mind the influence of the bulky anomeric substituents in nucleosides and nucleotides. Computational approaches to these problems through DFT methods for the isolated molecules are reported, and with the notable exception of α -D-lyxofuranoside, the gas-phase conformations are remarkably similar to those observed in the crystal structures. However, it is interesting to note that the energy-minimized structures for the isolated α -D-lyxofuranoside contain an *intramolecular* hydrogen bond, which appears to compensate for the strain induced by eclipsed ring substituents in these conformations.

Reviewed by Judith A.K. Howard, Chemistry Dept, U. of Durham, UK

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Jeffrey, G.A. & Mitra, J. (1983). *Acta Cryst.* **B39**, 469-480.
Marzec, C. J. & Day, L. A. (1993). *J. Biomol. Struct. Dyn.* **10**, 1091-1102.

IUCR ACTIVITIES

The powder world



The microstructure of materials and measurements of imperfections ranging from point defects and short-range disorder on the nanometer scale to residual stress and texture effects on the macroscopic scale are the focus of Newsletter 24 of the **IUCr Commission on Powder Diffraction**. Topics addressed include residual stress in thin layers (Welzel, Leoni, Lamparter and Mittemeijer) and individual grains (Poulsen and Kvik), size and size-strain effects in line broadening (Langford and Ungar), low-resolution and high-resolution diffraction experiments (Fewster), local and long-range order (Billinge, Petkov and Proffen) and modeling of microstructure in Rietveld refinement (Popa, Scardi, Leoni and Dong). Current microstructural analysis benefits from more accurate modeling techniques and significant improvements in radiation sources. Many of today's Rietveld-refinement programs can handle effects of texture line shift and broadening at an advanced level, which allows determination of pole figures, orientation-distribution functions, residual elastic stress/strain tensors, and locally varying lattice strains. The interdependence of sophisticated analysis methods, fast computers, and advanced instrumentation, is stimulating rapid advances in knowledge about the microstructure of materials.

D. Balzar (CPD News, No. 24, 2000)

Reference Materials: The certification of two new Standard Reference Materials (SRMs) by NIST will be of interest to powder diffractionists. The SRM640c (Silicon powder) and SRM660a (LaB₆ powder) standards will be valuable to Line Profile Analysis (LPA) and for the testing of instrumentation and methods. Applications and methodological developments in Powder Diffraction will be the subject of forthcoming meetings on Accuracy in Powder Diffraction III (Gaithersburg, MD, USA, April 22-25, 2001) and Size-Strain III (Trento, Italy, Dec. 2-6, 2001).

Powder Commission Officers (1999-2002). Chairman: P. Scardi (paolo.scardi@ing.unitn.it); Secretary: A.N. Fitch (fitch@esrf.fr); R. Delhez (Netherlands), S.P. Sen Gupta (India), R.B. Von Dreele (USA), D. Balzar (USA), G.J. Kruger (S. Africa), H. Fjellvåg (Norway), W.I.F. David (UK), R.E. Dinnebier (Germany).

CPD Projects: Information on the current status of the CPD projects is available at www.iucr.org/iucrtop/comm/cpd/projects/index.html. Size/Stain Round Robin: www.boulder.nist.gov/div853/balzar/s-s_rr.htm. Quantitative Phase Analysis Round Robin: www.iucr.org/iucr-top/comm/cpd/QARR/index.html.

P. Scardi (CPD News, No. 24, 2000)

MEETING REPORT

2000 Annual Meeting of CrSJ: IUCr President in Japan



Noriyoshi Sakabe: Let us keep a pioneer spirit!

The Annual Meeting 2000 and General Assembly of the Crystallographic Society of Japan was held in Sendai, Japan from Nov. 21-23, 2000. The meeting featured two plenary lectures, 205 oral and poster presentations covering all aspects of crystallography, an industrial exhibition and a special symposium marking the 50th anniversary of the CrSJ. Over 350 crystallographers attended.

In his plenary lecture *Structure Determination of Molecular Crystals Directly from Powder Diffraction Data*, K.D.M. Harris (Birmingham, U.K.) described structure solution using the Genetic Algorithm. In her plenary lecture *The structure and function of a highly proficient enzyme: orotidine 5'-monophosphate decarboxylase (ODCase)*, S. Larsen (Copenhagen, Denmark) discussed the unique arrangement of completely conserved lysine and aspartate residues in the enzyme.



Opening a cask of Sake with wooden hammers, which is a traditional Japanese ceremony to start a banquet. Left to right: Kenneth D.M. Harris, Henk Schenk, Fujiko Iwasaki, Sine Larsen, and Makoto Hirabayashi.

In the 50th anniversary symposium, 12 young and 4 senior crystallographers presented lectures on cryogenic protein crystallography (M. Nakasako, U. of Tokyo), analysis of cytochrome c oxidase (E. Yamashita, Osaka U.), neutron crystallographic analysis of DNA and hydration networks related to genetic information (T. Chatake, Japan Atomic Energy Research Inst.), small angle scattering with synchrotron radiation (T. Fujisawa, RIKEN), rapid crystal structure determination (H. Uekusa, Tokyo Inst. of Technology), photofunctional molecular materials (T. Yamada, Kyushu U.), magnetic conductors (H.

Fujiwara, Inst. for Molecular Science), micrometer sized single crystal analysis in materials science (Y. Kojima, Mitsubishi Chemical Corp.), electron diffraction (K. Tsuda, Tohoku U.), accurate structure by synchrotron X-ray diffraction (E. Nishibori, Nagoya U.), orbital ordering of YTiO_3 observed by resonant X-ray scattering (H. Nakao, KEK-PF), *ab-initio* structure determination from synchrotron radiation powder diffraction (S. Yamazaki, INAX Corp.), the future of X-ray, SR, neutron diffraction and structural physics (Y. Noda, Tohoku U.), structures of earth and planetary materials (T. Yamanaka, Osaka U.), the future of chemical crystallography (K. Toriumi, Himeji Inst. of Technology), and keeping a pioneer spirit (N. Sakabe, Foundation for Advancement of Int'l Science).

At the General Assembly, IUCr President H. Schenk presented a congratulatory message for the 50th anniversary of CrSJ. The banquet was held at the Special Guest House of historic Sake brewer, *Shozann-kan*.

A full program of the meeting can be viewed at the CrSJ website wwwsoc.nacsis.ac.jp/crsj/index-e.html. The Local Chair was Y. Noda (Tohoku U.) and the Program Chair M. Terauchi (Tohoku U.).

Masaki Takata, Nagoya, Japan

AWARDS AND PRIZES

Annual CrSj awards to Sasaki and Ito



Masahisa Ito, Henk Schenk and Satoshi Sasaki

Satoshi Sasaki (Tokyo Inst. of Technology) and Masahisa Ito (Himeji Inst. of Technology) received the 2000 CrSj Awards for their pioneering research using synchrotron radiation. Dr. Sasaki's most distinguished accomplishments have concerned the study of charge density and mixed-valence state of transition metal oxides by anomalous dispersion diffraction techniques. Dr. Ito developed synchrotron radiation magnetic scattering methods and measured accurate magnetic form factors of Fe and Dy.

NOTICE

Crystallographic training in Cairo

The first single crystal diffractometer in Egypt is now fully operational at the National Research Center in Cairo under the supervision of I. Farag and N. Aahme. This facility together with a well equipped powder diffraction laboratory directed by Karimat El-Said at Ain Shame Unwenti, Cairo, provide the basis for graduate education and training in X-ray crystallography for students from Africa and the Middle East. Students will require sponsorship and financial support for article sources such as UNESCO.

REGIONAL NEWS

10th Anniversary of the German Society of Crystallography (DGK)

10th Anniversary of the German Society of Crystallography (DGK)



Heinz Schulz



Ursula Steinike

The formal separation of German crystallographers dates back to 1965, when the Deutsche Vereinigung für Kristallographie (VFK) was founded in East Germany and the former East German Academy of Sciences ended cooperation with the German National Committee for Crystallography. During the 7th Congress and General Assembly of the IUCr in 1966 (Moscow) the German Adhering Body was divided into two regional committees. East Germany was granted separate representation in the General Assembly, which was then approved by the 8th General Assembly in 1969. It was not until the reunification of Germany on Oct. 3, 1990, that crystallographers in East and West could come together in a joint society, which was founded in Munich, Mar. 12, 1991, as the Deutsche Gesellschaft für Kristallographie (DGK) incorporating members of the former West German 'Arbeitsgemeinschaft Kristallographie' (AGKr) and of the East German VFK. Ten years later the DGK is a vibrant body with 17 active working groups covering the whole field of modern crystallography (www.kristall.ethz.ch/DGK). On the occasion of the 10th Assembly held in Bayreuth this year, the first president of the DGK, Heinz Schulz (Munich), and the last president of the VFK, Ursula Steinike (Berlin), were elected Honorary Members of this society.

Peter Paufler

MEETING REPORT

Powder diffraction schools

Venezuela. Two X-ray Powder Diffraction Schools were conducted at the Lab. Nacional de Difraccion de Rayos-X (LNDR-X), U. de Los Andes (ULA) in Merida, Venezuela during 2000, under the auspices of the National Lab. Program of CONICIT, the Venezuelan Science and Technology Office.

The school of Characterization of Polycrystalline Materials (**Jan. 24-28**) included lecturers on the fundamentals of structural analysis and microstructure characterization of materials. Invited lecturers included R. Jenkins (ICDD), R.L. Snyder (Ohio State U., USA), J.A. Henao (U. Industrial de Santander, Colombia), R. Atencio and R. Guevara (IVIC), J.R. Marcano and R. Guevara (UNEXPO) and members of the crystallography Group of ULA (M. Delgado, A. Mora, G. Díaz De Delgado, B. Ramirez and G. Delgado).

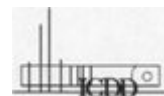
The school of Structure Determination and Refinement (**May 2-5**) included lectures by A. Fitch (ESRF, France), Jose Antonio Henao (U. Industrial de Santander, Colombia), R. Atencio, R. Vargas (IVIC), R. Guevara (UNEXPO) and members of the Crystallography Group of ULA. The majority of attendees were graduate students and young scientists from Venezuela and Colombia. For details contact M. Delgado, LNDR-X, U. de Los Andes, Fac. de Ciencias Apdo. Postal 40, La Hechicera. www.ciens.ula.ve/~Indrx.

Germany. A Workshop on Structure Determination and Refinement was held at the U. of Bayreuth, Germany (Oct. 2000).

Brazil. J. Faber & E. Ryba conducted an ICDD workshop, VII Latin-American Seminary of Analysis by X-ray Techniques, in San Pedro (**November 2000**).

MEETING REPORT

ICDD hosts annual X-ray clinics



Two week-long sessions in X-ray fluorescence and in X-ray diffraction were presented in **May 2000** to both new and experienced users working in academic, industrial, and government environments. The clinics offered students the opportunity to learn the principles and practices of these disciplines from some of the pioneers and leaders in the XRD and XRF fields.

MEETING REPORT

BCA: Non ambient condition

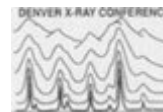


The British Crystallographic Assn (BCA) Industrial Group held a workshop on controlled environments in **June 2000** at Birkbeck College, chaired by D. Taylor (djttaylor@lineone.net) and J. Cockcroft (cockcroft@img.cryst.bbk.ac.uk). The workshop covered high and low temperature X-ray diffraction techniques (HTXRD), instrumentation and environment stages (M. Vickers); data handling (A. Jupe) and the use of synchrotron/neutron sources to study *in-situ* dynamic processes. The programme was presented via Microsoft PowerPoint and Internet web pages. Factors influencing the development of HTXRD were discussed, including sources and X-ray optics, solid state electronics detectors, and automation through computers. Reasons to employ the techniques are chemical (oxidation, reduction, corrosion, hydration, phase transitions, reaction kinetics) and physical (crystallite size, thermal expansion, strain, reorientation, heating and induction methods).

J. Kelly, BCA Newsletter, No. 75, December 2000

MEETING REPORT

Denver conference 2000



Three hundred and fifty attendees and 210 exhibit staff filled the conference rooms at the Marriott Tech Center for Denver Diffraction 2000, held **July 31-Aug. 4**. The Birks Award went to Y. Gohshi (Nat'l Inst. for Environment Studies, Tsukuba, Japan) for outstanding contributions to x-ray spectroscopy. The McMurdie Award, new in 2000, was awarded to G.J. McCarthy (N. Dakota State U., Fargo, ND) recognizing distinguished contribution to the Powder Diffraction File. The Jerome B. Cohen Student Award was presented to S. Vogel (Kiel U., Germany) for his paper entitled 'Non-destructive *In-situ* Real Time Measurements of Structural Phase Transitions Using Neutron Transmission'.

MEETING REPORT

Singapore software workshop



A group of participants for the SHELXTL workshop along with Ludger Häming and J.J. Vittal.

A five-day workshop and training course on crystallographic software programs was conducted at the X-ray Diffraction Lab of the National U. of Singapore by Ludger Häming, Bruker AXS, Germany, **Oct. 16-20, 2000**. Two days devoted to the SHELXTL software for structure solution, refinement and preparation of figures and tables were attended by more than 40 novice users, and 20 postgraduate students were given hands-on tutorials in the X-ray Diffraction Laboratory. This was followed by a three-day training session for advanced users on various aspects of the single crystal X-ray diffractometer SMART APEX CCD.

J.J. Vittal

MEETING REPORT

ACA 2000, St. Paul student views



Comments from recipients of the ACA 2000 travel grants



As a graduate student new to the field of crystallography, I was struck by the breadth of scientific research that utilizes the technique. From small-molecule to macromolecule crystallography, through technical advances in synchrotron radiation, I was stunned by the number of different lenses through which scientists see crystallography. Who would have predicted that a crystallography conference could double as a 5 day crash course in biology?

Raquel Lieberman, Northwestern U.



The feedback that I received from my poster presentation was incredible. Everyone was very supportive and offered valuable suggestions for future research. Prior to attending the ACA meeting I had been planning to apply to medical school. However, when I returned from the meeting I realized that I was not yet ready to give up research and I am now planning to pursue some sort of graduate work in the biomedical field when I graduate this spring.

Andrea Jorjorian, College of Wooster



I was particularly keen on talks exploring the direct applications of X-ray crystallographic methods in the design of drug molecules. It was an inspiring experience to meet and talk to people who belong to the crystallographic Hall of Fame, particularly Lyle Jensen, whose beautifully written 'X-ray structure determination', co-authored with George Stout, helped me to understand a number of abstract concepts in X-ray crystallography.

Eliud Oloo, U. of Saskatchewan, Canada



I obtained advice that has definitely accelerated the completion of my project. Thank you Dr. Stanfield and Dr. Greasley.

Johanna Mazlo, U. of Nebraska

..... I especially enjoyed the discussions with twinning experts Bob Sparks and Vic Young about my quadruply twinned crystal problems.

Sean X. Ouyang, Texas A&M U.



I was quite surprised by the extent of macromolecular crystallography in the meeting. For me personally, it was very important to participate in such a meeting, for I am 'on the way' from small to large molecules. The meeting exhibitions provided direct contact with companies working in the field. I found, in particular, very interesting and helpful information about 'Conquest', new software from Cambridge Crystallographic Data Centre. After the meeting I started to use it successfully at my home university.

Igor Fritsky, U. Heidelberg, Germany



At first glance, I found myself in a 'wrong' place where macromolecules dominate crystallography (some people complain about this). On the other hand, it was a nice chance to be stimulated in another environment where I can design my version of experiments and analyses. I believe many young scientists, including myself, enjoyed exposure to the variety of crystallography provided by the Poster Preview session, organized so well by Jeff Habel.

Yongjae Lee, SUNY Stony Brook



I met people from academia and industry, and was able to discuss the differences in the two career environments. The employment outlook session put on by the Young Scientist SIG was full of valuable information. I am always surprised by the friendly people at ACA meetings. It's not like that at every meeting you go to.

Joanna Clark, U. of Nebraska



I entered my poster with the hope for helpful comments, and with the ACA travel award, I was able to actually show up in St. Paul to hear such advice - from people such as Alexander McPherson, Robert Sweet, Bob Cudney, Don Voet, Lisa Edberg, and Kris Tesh. And while great progress was made on the research end, the ACA meeting was also filled with endless fun - booze and dancing at the MSC dinner. Greeting Snoopy around every corner, harassing the genetics activists, and reminiscing about Howard Hughes. One thought still lingers...is anyone going to answer Wim Hol's question 'Mr. Steitz, how do you think life was created in light of your ribosome structure?' Guess we'll all have to show up in Los Angeles to find out.

Chris Bunick, Vanderbilt U



The conference provided a lot more than an interesting collection of presentations. For example, unlike most I got to see Dr. BC Wang's rendition of YMCA at the MSC dinner. Shhh! Don't tell anyone but I escaped from the confines of the macromolecular world and I spent the evening with the small molecule group at the Mentor/Mentee dinner.

Jeff Lovelace, U. of Toledo

MEETING REPORT

International School on Crystal Growth



Lecturers at the Crystal Growth School in Trieste (left to right), H. Strunk, P. Rudolph, K. Byrappa, N. Ekins-Daukes, R. Fornari (Director of the school), L. Sorba (Secretary of the school), T. Boeck, D. Palmer. The Int'l School on Crystal Growth of Materials for Energy Production and Energy-saving Applications was held at the Abdus Salam Int'l Centre for Theoretical Physics (ICTP) of Trieste (Italy) **March 5-10, 2001**. The main objective of this school for PhD and Master students was to provide an overview of classical and modern growth technologies and lectures on crystal growth of energy-related materials. Three main classes of materials were considered: materials for energy conversion (solar cells, thermo-photovoltaic converters), energy storage (carbon nanotubes and superconductors) and energy saving (superconductors, soft magnets for low-loss transformers, nitrides for visible and white light LEDs). Lectures on structural and electrical characterization were also included, bearing in mind the important role that extended and point defects play in material characteristics and device performance.

The school was attended by 40 participants (from Italy, Eastern and Western Europe, Northern Africa, South America and Asia). The truly international character of ICTP and the friendly behaviour of participants and lecturers provided a stimulating atmosphere for discussions. Two afternoon sessions devoted to short, informal presentations by 24 students generated new contacts and strengthened relations among participants.

The school was promoted by the IUCr Commission on Crystal Growth and Characterization of Materials and sponsored by the IUCr, Italian Crystallographic Assn (AIC), Italian Group for the Structure of Matter (GNSM-CNR), and Abdus Salam Int'l Centre for Theoretical Physics.

A detailed report is available at www.maspec.bo.cnr.it/ut/d11200/NEWS/trieste/report_school.htm.

R. Fornari, Director of the School

MEETING REPORT

Sagamore XIII, Poland

The Sagamore meetings focus on aspects of charge, spin and momentum distributions, their determination from a wide variety of experimental techniques, and their detailed analysis and comparison with theory. Sagamore meetings provide an opportunity for scientists from different disciplines to meet and lead to closer collaboration and mutual understanding and appreciation of one-another's science.

Particular highlights of Sagamore XIII (Stare Jablonki, Poland, **Sept. 3-9, 2000**) included talks by F. Tasset (ILL) on spherical neutron polarimetry (which promises to enable solution of magnetic structures that were previously intractable), W. Jauch (Hahn-Meitner Inst.) on the benefits of gamma radiation (in particular he presented evidence that the long-standing discrepancy between X-ray and neutron ADPs is due to the use of graphite-monochromated Mo radiation, and detailed studies on extinction which strongly corroborated the standard Becker-Coppens model), A. Shukla (ESRF) on Compton scattering (which was claimed to be more sensitive to intermolecular interactions than conventional charge density studies).

The IUCr Commission on Charge, Spin and Momentum Densities was formed in 1975 as an outcome of the Sagamore meetings, and to this day the CSMD Commission is actively involved in the planning and execution of these conferences. Sagamore XIV will be held mid-August 2003 on an island off the southern Queensland coast.

Mark Spackman, U. of New England, Soc. of Crystallographers in Australia and New Zealand Newsletter, No. 47, Nov. 2000

MEETING REPORT

Indo-French workshop on weak intermolecular interactions



Cosmetics in ancient Egypt: Chemistry as a subject is a lot older than one might think and there is now definite evidence that the ancient Egyptians were proficient in synthetic techniques enabling them to make lead compounds which they then used for eye make-up (Courtesy of G. Tsoucaris, Louvre Museum, Paris).

Thirty scientists participated in an Indo-French workshop on 'Static and dynamic aspects of weak intermolecular interactions' in Hyderabad, **Feb. 17-21, 2001**. The workshop, sponsored by the Indo-French Centre for the Promotion of Advanced Research (CEFIPRA) and organised by G.R. Desiraju (Hyderabad) and P. Batail (Nantes) brought together chemists, crystallographers, physicists, biologists and theoreticians for a discussion of weak hydrogen bonds and other intermolecular interactions in the static and dynamic context and included sessions on crystal engineering, intermolecular interactions, theoretical and computational approaches, and inorganic and biological systems. C.N.R. Rao (Bangalore) described the self-assembly of complex and exotic open-framework inorganic materials and argued that the mesoscopic assembly of 1D and 2D arrays and 3D superlattices in metal nanocrystals is governed by the Aufbau principle.



Participants of the Indo-French workshop on weak intermolecular interactions in February 2001. G.R. Desiraju described the significance of multi-point recognition supramolecular synthons. M.W. Hosseini (Strasbourg) showed molecular networks assembled using programmed tectons and specific interaction patterns. A debate on the meaning of the terms, tecton and synthon followed: a tecton is a molecule with potential hydrogen bonding sites on its periphery, and a synthon is an intermolecular interaction pattern of functional groups and contains only parts of molecules. The organization of amphiphilic lipid molecules at the air-water interface (P. Ganguly, Pune), dynamics of C-H...O interactions in trimethyl isocyanurate (K. Boubekour, Nantes), nonlinear optics and multipolar engineering with 2D and 3D octupolar molecules (J. Zyss, Paris), weak van der Waals interaction effects on the atomic and mesoscopic scale (P. Levitz, Palaiseau), molecular dynamics simulations on atomic argon at the solid-liquid transition temperature (R. Ramaswamy, New Delhi) and the static and dynamics of cooperative phenomenon in neutral-ionic phase transitions (H. Cailleau, Rennes) were described and discussed. Exploring weak interactions based on topographical characteristics of molecular electrostatic potential by S.R. Gadre (Pune) was followed by a lecture by E. Candell (Bellaterra, Spain) on the relationship between the crystal and electronic structures in BEDO-TTF salts. D. Mukherjee (Calcutta) proposed a method to treat inter-fragment interactions in the presence of valence fluctuations and B. Bagchi (Bangalore) spoke about dynamics of tagged water molecules and cesium ions at the aqueous micellar surface.

A visit to 400-year-old monuments was followed by the lecture of G. Tsoucaris (Paris) on the chemistry of cosmetic materials in ancient civilizations. From Greco-Roman texts and powder X-ray diffraction patterns, it appears that laurionite (PbOHCl) and phosgenite ($\text{Pb}_2\text{Cl}_2\text{CO}_3$) were synthesized by the Egyptians in 2000 BC for use as eye make-up and may have had religious connotations (see Figure).

P. Batail discussed the interplay of hydrogen bonding and redox states in EDT-TTF-amides. A. Nangia (Hyderabad) showed that the halogen... π synthon induces crystallization in a polar, non-centrosymmetric space group while M. Fourmigué (Nantes) discussed the interplay of halogen and hydrogen bonding in TTF molecules. This led to a discussion of what controls crystal packing — shape or interaction? R. Ziessel (Strasbourg) correlated ferromagnetic interactions in nitroxide radicals with C-H...O hydrogen bonds in their crystal structures. K.N. Ganesh (Pune) showed intricate hydrogen bond patterns in crystalline adducts of cyanuric acid and adenine derivatives.

The session on inorganic systems featured discussions of d^0 transition metal oxides with unique properties (J. Gopalakrishnan, Bangalore), weak interactions in copper and silver coordination complexes (M.V. Rajasekaran, Hyderabad), hydrolytic polycondensation materials (G. Cerveau, Montpellier), and a Monte Carlo simulation of the dynamics of aromatic guests in a zeolite channels (J.A.R.P. Sarma, Hyderabad).

In a session on weak macromolecular interactions, the role of C-H...O and C-H... π interactions in stabilizing enzyme crystal structures (M.A. Viswamitra, Bangalore), the stereochemistry of aromatic residues in protein complexes (P. Chakrabarti, Calcutta), crystallization of proteins on carbon nanotubes (C. Mioskowski, Illkirch), free energy contributions to DNA-protein and drug-protein binding (B. Jayaram, New Delhi), and an overview on enthalpy-entropy balance in ligand-receptor interactions (B. Gopalakrishnan, Chandigarh) were discussed.

The atmosphere was lively and informal and the discussion prompted serious thought about the static and dynamic consequences of weak intermolecular interactions.

Ashwini Nangia, Hyderabad, India and Marc Fourmigué, Nantes, France

NOTICE

Bruker AXS and Nonius unite



Sales and support visiting the Karlsruhe location (left to right) Eric Hovestreydt, Paul Ulrich Pennartz, and Frank van Meurs.

After talks extending back more than two years, the Nonius crystallography business of Delft Instruments agreed to join with Bruker AXS worldwide on April 10, 2001. The combined crystallography product lines of Nonius and Bruker AXS will be marketed under the joint brand Bruker Nonius. The combined user instrument base includes more than 1,000 four-circle diffractometers and over 400 CCD instruments for single crystal diffraction.

Both instrument companies are deeply rooted in crystallography. Nonius began as a mechanical instrument business in 1948, and merged with Enraf in 1960 to form the Enraf-Nonius business many users remember well. In 1990, Oldelft acquired the combined business and subsequently formed the current business unit, which was later renamed Nonius B.V. This unit now becomes Bruker Nonius B.V. and remains located in Delft, The Netherlands.

Bruker's X-ray roots reach back to 1896, when Wilhelm Conrad Roentgen ordered his first X-ray tubes from the predecessor company to Siemens. In 1927 Siemens introduced its first generation of analytical X-ray instruments. In 1969 the P1 four-circle diffractometer was introduced by the Syntex group headed by Dr. Robert Sparks, still with the combined company today in Madison. In 1984 Nicolet acquired this X-ray business, which was then merged with the Siemens diffraction and fluorescence products in 1989. By 1997 Bruker acquired this Siemens analytical X-ray business and created the Bruker AXS company as a complement to the Bruker NMR, mass spectrometry and optics businesses.

We are very excited about the new opportunities and challenges offered by this new alliance. However, we can imagine that this raises some questions about the present and the future! We want to assure the community that the current product lines of Nonius and Bruker AXS will continue to be fully supported. Software development plans in execution will continue as planned. Our combined obligations will be unconditionally respected.

All former Nonius and Bruker single crystal technical, manufacturing and support personnel have become part of the joint operation. The active development capacity and quality especially for crystallographic products will be strengthened at our three competence centers in Delft, Karlsruhe and Madison. Joint Bruker-Nonius teams are already integrated and have begun their work to develop even better solutions for the future, bringing us closer to the realization of a 'dream machine' for X-ray crystallography. Already we have a wider choice of products and accessories for crystallographic solutions in small molecules and biological macromolecules.

The joint organization includes a larger number of dedicated service and support specialists, and more service centers worldwide. The number of applications scientists available to assist with experiments has increased, and the specific application expertise becomes broader in nature. For the short term, we are moving very actively towards combining our user meetings. Nonius and Bruker users are invited to a combined user reception at the ACA meeting in Los Angeles, to the Cracow ECA meeting for a half-day user meeting, and to the Bangalore AsCA meeting. Our two web sites will provide updated information on these events, and will gradually grow towards an expanded information platform. Contact information by telephone, fax, email and web site addresses remain unchanged for the worldwide locations for both businesses. Please contact us with any questions - we look forward to exciting new developments in the near and distant future.

E. Hovestreydt (eric.hovestreydt@bruker-axs.de), F. van Meurs (vanmeurs@nonius.nl), and P.U. Pennartz (pennartz@nonius.nl) Bruker Nonius

NOTICE

Canadian institutes for health research

On June 7, 2000, the Canadian Institutes for Health Research (CIHR) was officially created to replace the Medical Research Council of Canada as the primary funding source for health research in Canada. The objective of CIHR is to excel in the creation of new scientific knowledge and its translation into more effective health services and products and a strengthened health care system. The Institutes will encourage interdisciplinary health research and forge a health research agenda across disciplines, sectors, and regions. Each Institute will include fundamental bio-medical research, clinical research, and research on health systems and health services, societal and cultural dimensions of health and environmental influences on health. Each mandate profiles the research areas around which the Institute can focus, develop and evolve. (www.cihr.org/index.shtml)

From the ACA Newsletter, Winter 2000

NOTICE

NIST centennial celebration

The Centennial Celebration of the Nat'l Inst. of Standards and Technology (NIST), formerly the Nat'l Bureau of Standards (NBS), takes place in the year 2001. NIST has made significant contributions to the advancement of the fields of crystallography, biology and materials science. The research has been carried out as a fundamental part of the overall mission of NBS/NIST and has become an integral part of many aspects of its research programs. Eleven pages of the *Winter ACA Newsletter* were devoted to articles written by NIST crystallographers describing past accomplishments and current activities. The articles cover a broad spectrum of topics including structural databases, high-pressure crystallography, neutron crystallography, structure determination via neutron and x-ray diffraction, quasicrystals, reduced cells, magnetic structure determinations, polymer crystallography, electron diffraction, properties of materials databases, protein crystallography, novel biomaterials, biological minerals, crystallography of construction materials, and synchrotron radiation. There will be a one-day symposium honoring the NIST centennial at the ACA 2001 meeting in Los Angeles.

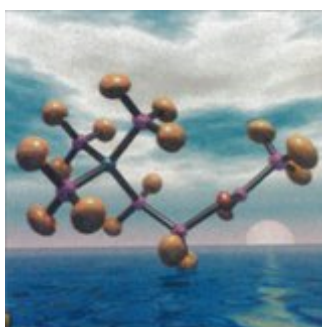
NOTICE

Art with small molecules competition

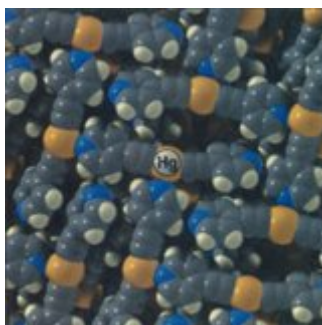


Cecil Simpson's 'The Seascape' won first place in the WOW-2000 Art with Small Molecules Contest sponsored by the Small Molecule Special Interest Group (SIG) of the American Crystallographic Assn. Submissions for the WOW-2001 competition are encouraged and can be sent to wow@bernstein-plus-sons.com.

The first place entry was a photomicrograph taken at 70X by Cecil Simpson (Lubbock, TX, USA) with a stereo Olympus microscope using cross polarization. The 'birefringent' crystals were obtained using small quantities of 9-fluorenone mixed together on a microscope slide and melted using an alcohol lamp. A cover glass was placed on the clear liquid and the material allowed to cool at room temperature. The resulting crystals were then photographed.



The second place entry, 'Nanodali', was a POVRAY drawing of acetylcholine rendered by Alastair Florence (Glasgow, Scotland) and submitted by Kenneth Shankland of Chilton.



The third place entry, 'T-shaped', was a Chem-Ray drawing submitted by Joseph W. Lauher (Stony Brook, NY, USA) showing the crystal packing of mercury(II) bis(4-pyridylacetylide) from a structure determined by Lauher's graduate student Sean Curtis.

Herbert Bernstein

AWARDS AND PRIZES

ORTEP of the year - 2001

Richard Harlow

The R. Harlow Foundation for Disabused Crystallographers will, as usual, be presenting a check for \$200, at the Los Angeles ACA Meeting in July 2001, for the best example of how an ORTEP drawing was used to spot and resolve a 'problem' structure. Any published structure in a referred journal is eligible for submission, but the submitter must clearly demonstrate the manner in which ORTEP (or any thermal ellipsoid plotting program) was used to indicate that the structure as published was incorrect and must provide an ORTEP of the 'corrected' structure. Entries should be addressed to the Foundation at 7 Shull Dr., Newark, DE, 19711 USA. Details of two other Foundation initiatives, the Hydrogen Challenge and the Low-Temperature Prize, can be found under the ACA Service SIG web page at www.pitt.edu/~geib/aca.html.

R. Harlow

NOTICE

Women in science

In the editorial in *C & E News* in March 2000, Debra Rolinson cited the disparity between women earning a Ph.D. in chemistry and their representation on University faculties, and other data concerning inequitable treatment of women in science. She suggested it may be appropriate for the US government to withhold Federal support until the disparity is corrected. Rolinson's editorial received responses from understanding and sympathetic men (May 8, 2000). One said 'women scientists are among the most productive at *my* company and *my* university' and thinks quotas would diminish women's status. A second said 'we all know that men and women excel in different areas'. Apparently men just happen to be better at the jobs that are more powerful and pay better. The same issue of *C & E News* noted that of the top 75 chemical producers in the US not one has a female chief executive officer, chief operations officer, or chief financial officer.

C&E News, March 2000

NOTICE

Bacteria silver lined

The synthesis of silver crystals by a bacterial strain, *Pseudomonas stutzeri*, originally isolated from a silver mine has been reported (*Proc. Nat'l Acad. Sci.* **96**, 13611-13614, 1999). Tanya Klaus found that by culturing the bacteria in the presence of high concentrations of silver salts, they could create crystals of well-defined compositions and shapes in the region surrounding the plasma membrane. The 200 nm size of the crystals suggests that they might eventually be used for the formation of thin metal films to absorb solar energy or to construct nanometer scale materials with unique optical and electrical properties useful in microelectronic applications.

Nature Biotechnology, January. 2000

NOTICE

Going 3D

A French biotech start-up plans to launch an international consortium aimed at revealing the three-dimensional crystal structure of 100 cell membrane proteins, many of which could be promising drug targets. The 3-year, \$9.3 million project, led by BioXtal in Roubaix, France, has the support of 18 major pharmaceutical companies including Roche, Novartis, Glaxo-SmithKline, AstraZeneca, Merck KGaA, Genencor, Takeda, and four academic labs in France, Germany, and the Netherlands. This initiation is the first to focus on membrane proteins. The targets will be 'G' protein-coupled receptors.

Science Vol. 291, February 2001

AWARDS AND PRIZES

Fankuchen award to Stewart



James McDonald Stewart is the 2001 recipient of the Fankuchen Memorial Award, which recognized an outstanding crystallographer who is known to be an effective teacher of crystallography. Jim had a distinguished teaching and research career at the U. of Maryland. His career spanned the era in which the way that crystal structures were solved underwent a profound change. As the major developer of the XRAY and XTAL crystallographic software packages, Jim was an outstanding innovator in large-scale computing techniques. His software packages were benchmarks for crystallographic computing and data standards, and influenced the design of software in other scientific disciplines including computational chemistry. He was a leader in the implementation of computer applications to all aspects of crystallographic research - from powder to proteins. He popularized computational approaches through his contributions to the ACA and IUCr teaching and computing schools. He was the quintessential teacher: well-informed, intellectually curious, clear in his explanations, patient with students, and inspiring to young scientists. His zest for his subject was communicated in every interaction, whether it was an explanation of space groups, the mechanics of a fast Fourier transform, or the arcana of data structures that would be transportable across computing platforms. By creating the first comprehensive, transportable, and integrated system of crystallographic programs (The XRAY System), he revolutionized the field of crystallography. With a 'user friendly' system with one program flowing smoothly to the next, the crystallographers could solve a broad spectrum of structures from start to finish. Jim Stewart's immense lifetime contributions to the development and teaching of computing methodologies have played a major part in the success and prominence that crystallography holds in science. His educational influence has reached far beyond the conventional classrooms. The Fankuchen Memorial Award, an appropriate recognition for these most important contributions, will be presented to Jim Stewart at the ACA meeting in Los Angeles, July 21-26, 2001.

Students, Colleagues and Friends of Jim Stewart

AWARDS AND PRIZES

Megaw honored



Helen Megaw (who celebrates her 94th birthday in 2001) received an honorary degree from Queen's U., Belfast, Northern Ireland, July 7, 2000. Dr. Megaw, a native of Northern Ireland, attended Queen's before earning BA and PhD degrees from the U. of Cambridge. One of the pioneers in the field of crystallography, her PhD concerned the structure of ice. After postdoctoral work in Vienna and Oxford, she taught in girls' schools in England and worked in an industrial research laboratory. After the second world war she worked in the Cavendish Laboratory in Cambridge on ferroelectric crystals, wrote the book 'Ferroelectricity in Crystals', and did pioneering work on disorder in crystals and its effect on the x-ray diffraction patterns. She was awarded the Roebling Medal of the Mineralogical Society of America in 1989. An island in the Antarctic is named after her in recognition of her work on ice. She returned to Northern Ireland when she retired from the University of Cambridge in 1972. Further information can be found in the American Inst. of Physics History of Physics web pages www.aip.org/history.

AWARDS AND PRIZES

Hawthorne awarded chair



Frank C. Hawthorne, Distinguished Professor of Geological Sciences at the U. of Manitoba, has been awarded a Canada Research Chair in Crystallography and Mineralogy by the Natural Sciences and Engineering Research Council of Canada. This provides teaching relief and significant additional research funding for seven years. Frank is an authority on amphiboles and other groups of complex rock-forming minerals, the topology and energetics of mineral structures, long-range and short-range order in minerals, the role of light lithophile elements in complex minerals, crystal-structure determination of minerals, and complementary analytical techniques. He has described many new minerals, interacting widely with the mineral-collecting community in the process. His work addresses some of the most fundamental questions on the behaviour of solids in general and minerals in particular.

NOTICE

News of crystallographers

Distinguished lecturers

The Mineralogical Soc. of America Distinguished Lecturer Program 2000-2001 Tours will feature speakers: I. Parsons, J. Holloway and R. Jones. For more information visit www.minsocam.org/MSA/The_Lecture_Program.html.

To celebrate the U. of Manchester's 150th anniversary, J.R. Helliwell presented the keynote lecture 'X-ray Crystal Structure Analysis and Manchester: from W.L. Bragg to the Present Day' on Feb 5, 2001. *BCA Newsletter, December 2000, No. 75*

Distinguished Fellows

The list of current Biophysical Society Fellows includes C. Cohen, D. Eisenberg, M.G. Rossmann, R.M. Stroud, H.M. Berman, D.L.D. Caspar, F.M. Richards.

New Fellows of the American Assn for the Advancement of Science include: S.R. Sprang, C. Stauffacher, and G. Wagner. *AAAS News, October, 2000*

Editors

D. Voet, U. of Pennsylvania, and J.G. Voet, Swarthmore College, the new co-editors-in-chiefs of the IUBMB *Journal of Biochemistry and Molecular Biology Education*.

ACA Officers

President: W. Stallings, Vice-President: C. Carter, Jr., Secretary: L. Brammer, Treasurer: D. Ohlendorf, Biological Macromolecules: C. Abad-Zapatero, Fiber Diffraction: D. Kirschner, General Interest: G. Borgstahl, Neutron Scattering: S. Billinge, Service Crystallography: P. Boyle, Small-Angle Scattering: P. Butler, Small Molecules: J. Bollinger, Young Scientists: N. Silvaggi.

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BOOK REVIEW

Books

Dynamic Theory of X-Ray Diffraction [André Authier, 2001, Hardbound, 640 pp, £85.00, Oxford Univ. Press]. Dynamical theory has seen exciting developments since the advent of synchrotron radiation. This book, an up-to-date account of the theory of diffraction and its applications, includes an introduction to the subject, an account of early developments and basic results, detailed development of the diffraction and propagation properties of x-rays on perfect crystals and extension of the theory to deformed crystals. Three applications of the theory are discussed in detail: x-ray optics for synchrotron radiation, locations of atoms at surfaces, and x-ray diffraction topography. The book includes more than 1,200 references to the literature, and will be a useful reference work for lecturers, graduate students, and researchers. (www.oup.co.uk)

ECM 18 proceedings

Materials Structure in Chemistry, Biology, Physics and Technology [vol. 6, no. 2, 1999, 87 pps] includes 22 reviewed papers on special topics presented at ECM-18.

Advances in Structure Analysis [Editors: R. Kuzel, J. Hasek, 2000, 510 pages, Kluwer Academic Publishers] Reviewed papers on special topics presented at the 18th European Crystallographic Meeting (ECM-18) including papers on materials structure and physics (9 papers), chemical crystallography (9 papers), structure determination (6 papers), biology (3 papers), and symmetry (2 papers). Authors include: J.W. White, P. Klmanek, H.J. Bunge, P. Barnes, C. Landron, Gu Nanju, R.I. Barabash, S.V. Starenchenko, I.V. Alexandrov, M. Steinhart, V. Kaucic, A. Le Bail, K.D.M. Harris, F.H. Herbststein, S.V. Krivovichev, G.A. Geguzina, P. Capkova, K. Yoshimura, K.S. Byram, D. Wigel, V. Kopsky, M.G. Mirceanu, A. Deriu, K. Vlahovicek, C.M. Weeks, A. Podjarny, C. Gilmore, V. Lamzin, C. Giacovazzo, V.Y. Lunin, and co-authors. (<http://krystal.karlov.mff.cuni.cz/xray>)



The Structures of Life. This free booklet is geared toward an advanced high school or early college-level audience and explains how structural biology provides insight into health and disease and contains a general introduction to proteins, a chapter each on X-ray crystallography and NMR, and a chapter on structure-based drug design. It also features “Student Snapshots” designed to inspire young people to consider careers in biomedical research. The Structures of Life and other science education booklets are published by the Nat’l Inst. of General Medical Sciences, a component of the NIH (USA). (www.nigms.nih.gov/news/publist.html)

Supramolecular conference

Current Challenges on Large Supramolecular Assemblies [proceedings of an Advanced Research Workshop (NATO), edited by G. Tsoucaris, Hardbound, 1998, 438 pp, EUR 179.50/USD 237.50/GBP 154.50] An interdisciplinary study of supramolecular assemblies in which several methodologies for structural characterization are combined. The chapters of this book aim at bridging areas of research of methods of investigation of supramolecular assembly. Crystal structures are studied within the framework of creating and characterizing organized entries in one, two and three dimensions. (www.wkap.nl/kaphtml.htm/ELECCAT) G. Tsoucaris (France)

Physics Today. Physics Today magazine has expanded its web site to include full editorial content from the magazine. The new redesign includes repackaging the articles into a more readable format for the web. 'We hope to expand the amount of materials on physicstoday.org to include papers from the magazine's archive,' says Paul Guinnessy, Physics Today's Online Editor. 'The December online edition of the magazine includes a collection of arms control articles from the past few decades'. The site is currently developing new services and restricted access controls. Access will remain free to subscribers and members of ACA and societies connected to the American Inst. of Physics (USA) (<http://physicstoday.org>)

FEATURE ARTICLE

Update on Protein Data Bank activities



The first annual report for the Protein Data Bank (PDB) describes the purpose and functions of the PDB, details accomplishments during this first year of Research Collaboration for Structural Bioinformatics (RCSB) management, and outlines plans for 2001. As the sole international repository for three-dimensional structure data of biological macromolecules, the PDB is an important resource for the entire life-science research community. The RCSB's mission is to enable new science. Each of the RCSB partner sites contributes to the operation and development of the PDB: Rutgers, data deposition and processing; Nat'l Inst. of Standards and Technology (NIST), data uniformity, exploring issues specific to nuclear magnetic resonance (NMR), and data archiving; and the San Diego Supercomputer Center (SDSC) at the U. of California, San Diego (UCSD), data query reporting and distribution. The RCSB has made great strides in enhancing the PDB due to its unique personnel, hardware, software and network infrastructure. The seamless transition of the PDB from Brookhaven Nat'l Laboratory was completed three months ahead of schedule, a large number of files were processed with a rapid turnaround time, legacy data were reprocessed and cross-referenced to ensure reliability, and an average of 90,000 hits per day have been accommodated by the main PDB web site alone. Plans for the future are to enhance the PDB's many features with new capabilities, including a higher, faster throughput of deposited data; a greater number of query capabilities, including more complex and accurate queries, and a more uniform archive.

Data Deposition

From July, 1999 to June, 2000, 2292 structures were deposited at the RCSB and 468 backlog entries and 456 'layer 1' entries were processed. The data rate during the period was on average 44 depositions per week. The average time to fully process an entry was less than 12 days. 81% are from x-ray experiments, 15% are from NMR experiments, 61% of data deposited are from North America, 25% from Europe, 11% from Asia, and 2.4 % from Australia. Proteins make up 89% of the depositions, while 11% are nucleic acids. Of the structures deposited, 20% were indicated by the author to be held until a particular date, 57% were indicated to be held until the publication of the corresponding article, and 23% were indicated to be released immediately.

A popular PDB feature, the Validation Server (ADIT), allows depositors to check a structure at any time during structure determination and refinement. It checks the format consistency of coordinates during the Precheck step, and creates validation reports about a structure before deposition using ADIT (<http://pdb.rutgers.edu/>). Once deposited, entries are processed to completion, returned to the author for review, and released on the PDB site (www.pdb.org/) and its mirrors. The PDB staff continues to enhance and upgrade the capabilities of the PDB searching and reporting tools. As part of the Data Uniformity project, PDB members have curated the *R*-factor, resolution data, and primary citation data for all entries in the PDB, and have incorporated this information into the database. These fields are available for improved searching, and the updated data are available via database reports.

Data Distribution

The site's 'Get Educated' page includes an introduction to proteins for general audiences and materials for undergraduates on topics such as nucleic acids, principles of protein structure, and electron microscopy. Tutorials are available on two popular molecular graphics viewing programs, how to query the PDB and how to use RasMol and the Swiss-PDB Viewer (Guex, Peitsch 1997). Links are frequently added to this resource, which also includes papers on the PDB, animated presentations about the PDB,

and VRML 'protein documentaries' developed by students. The electronic help desk at info@rcsb.org, which is available to answer all types of questions about the PDB, usually within a 24-hour period.

Other developments in query and reporting include expanded ligand searching and reporting capabilities, improved access to dynamic links using the Molecular Information Agent (<http://mia.sdsc.edu>), the accurate query of enzymes, the incorporation of cross-links to sequences databases, and improved graphics options. The PDB can now be queried based on source, by number of chains, and by the availability of experimental data.

Each month a key biological molecule is profiled as the Molecule of the Month. Beautiful images of the molecule are provided by D. Goodsell of the Scripps Research Inst. and featured on the PDB home page and links provide additional information about the structure and function of the molecule at a general level.

Usage, which grew in the initial months of operation, has now leveled off at about 90,000 Web hits per day and 70,000 PDB files downloaded per day.



The RCSB PDB Team (left to right): Phoebe Fagan, Dorothy Kegler, Haiyan Cheng, John Westbrook, Zukang Feng, Phil Bourne, Gary Gilliland, Diane Hancock, T.N. Bhat, Brad Kroeger, David Padilla, Victoria Colubesh, Helge Weissig, Narmada Thanki, Gnanesh Patel, Bohdan Schneider, Helen M. Berman, Nita Deshpande, Wolfgang Bluhm, Kyle Burkhardt, Lisa Iype, Ward Fleri, Christine Zardecki, Tammy Battistuz. The RCSB-Rutgers site also maintains two other sites: deposit@rcsb.rutgers.edu, for general deposition and processing questions; and help@rcsb.rutgers.edu, for ADIT information. Furthermore, the pdb-l@rcsb.org discussion list provides a forum for users to interact and collaborate. The PDB staff attends conferences, hosting exhibit booths, demonstrations, and user group meetings to gather feedback from the community and to provide information about PDB's capabilities and growth. In order to better serve the needs of the scientific community, the RCSB is collaborating with BioMagResBank (BMRB), Cambridge Crystallographic Data Centre (CCDC), European Bioinformatics Inst. (EBI), Inst. for Protein Research, Osaka Univ., Nat'l Ctr for Biotechnology Information (NCBI), NCI-Frederick Cancer Research & Development Foundation and the Swiss Inst. for Bioinformatics/Glaxo.

It is estimated that the PDB could grow to approximately 35,000 structures by 2005, nearly tripling its size. A major factor in this growth is structural proteomics, the determination of the structures of as many of the proteins as possible, in the shortest time possible. This increased volume will present a challenge to the PDB. As technology advances, the PDB's user base will also expand. In order to accommodate this demand, the RCSB plans to enhance the robustness of the PDB's query capabilities. The RCSB is proceeding with the next phase of archiving the physical data, which involves scanning and electronically storing all documents associated with the PDB. Data uniformity work will continue by focusing on structure classification, compound records, chain ID fields, refinement parameters, coordinates, sequence records, and the biological unit.

(taken from the PDB annual report July 1999-June 2000)

NOTICE

New tools at ISIS

OSIRIS The OSIRIS spectrometer, a new instrument at the ISIS Facility at the CLRC Rutherford Appleton Lab, was inaugurated on Oct.6. The OSIRIS will provide users with the powerful combination of a spectrometer and a diffractometer for measurement of structure and physical properties of a wide range of materials including electro-active polymers, energy storage systems and magnetic materials. The instrument combines high resolution at long d -spacing coupled with the highest count rate available today. The OSIRIS Project is an international collaboration involving Spain, Sweden, Switzerland, India, Italy, and two UK funding bodies, the Higher Education Funding Council (HEFCE) and the Engineering and Physical Sciences Research Council (EPSRC). More information is available at www.isis.rl.ac.uk/crystalanalysers/osiris/. *David Martin*

GEM The new General Materials diffractometer (GEM) at the ISIS neutron source was constructed by the Collaborative Research Group (CRG) headed by P. Day of the Royal Inst., and funded by EPSRC, the RIKEN lab. in Japan and the Higher Education Funding Council for England (HEFCE) through the Joint Research Equipment Initiative (JREI). The performance of this high flux high resolution diffractometer in its initial year has been impressive, allowing rapid data collections (under a minute) and permitting the study of small samples (3 mg). Details at www.isis.rl.ac.uk/disordered/gem/gem_home.htm. *C. Wilson*

BCA Newsletter, No. 75, December 2000

OBITUARY

Shizuo Miyake (1911-2000)

We regret to announce that S. Miyake, one of the leading figures in Japanese Crystallography, died recently at 88 years of age. He graduated from the U. of Tokyo, and started research predominantly on X-ray and electron diffraction, working for S. Nishikawa. In the late 1950's he was appointed to a Professorship at the Tokyo Inst. of Technology, and soon moved to the U. of Tokyo, Inst. of Solid State Physics. Until his retirement he was the Director of that Institute. He published numerous research papers, the most famous of which include: 'An experimental demonstration of domain structures of Rochelle salt by using the dynamical extinction effects in X-ray diffraction' and 'An experimental discovery of a failure of Friedel's law in electron diffraction'. He attended the IUCr Congress and General Assemblies, often as the head of the Japanese delegations, and served the IUCr as a co-editor of *Acta Crystallographica* and a commission member.

K. Ohashi (ogawa@ramie.c.u-tokyo.ac.jp)

OBITUARY

Joshua Ladell (1923-2000)

J. Ladell passed away in Jerusalem, Israel, on Jan. 28, 2000. He pursued graduate studies in Physics at the Polytechnic Inst. of Brooklyn, where he received the M.S. degree in 1951 and a PhD in 1954. His dissertation was completed under I. Fankuchen. Josh was the first to attempt a least squares crystal structure refinement using the computation facilities at the IBM Watson Lab. He was awarded a Lipsky exchange fellowship to spend 1954-1956 with Gerhardt Schmidt at the Weizmann Inst. of Science in Rehovot, Israel. W. Parrish recruited him to join Philips Labs in New York. His work included studies of the geometrical optics of single crystal diffractometers, applications of crystallography to fluorescence analysis instrumentation, the theory of instrumental diffraction profiles, the development of the PAILRED automated single crystal diffractometer system, the use of dedicated microprocessors to control X-ray diffraction instruments, and the use of forbidden reflections to solve the phase problem. He developed a generalized powder diffractometer, and with co-workers published two seminal papers on the determination of surface state electronic density in thermally oxidized silicon. Josh was a dedicated scientist, crystallographer, friend and colleague.

H. Steinfink, N. Spielberg (ACA Newsletter, Summer 2000)

OBITUARY

Harry Brumberger (1926-2000)



H. Brumberger, Professor of Chemistry at Syracuse U. and a pioneer in the field of small-angle scattering, died Nov. 10, 2000. Harry came to the US from Vienna, Austria with his parents, who were fleeing anti-Semitic persecution. His PhD in chemistry (1955) was directed by Rudolph Marcus, later a Nobel Prize winner in Chemistry. After his PhD he worked as a post-doctoral associate with Nobel Prize winner, Peter Debye at Cornell U. He joined the Chemistry Dept. at Syracuse U. in 1957 where he served as director of the Graduate Biophysics Program and of the Solid State Science and Technology Program. Harry became an expert in small angle scattering and he organized the first international conference on the topic in Syracuse, and a NATO Advanced Inst. on Small-Angle Scattering in Como, Italy in 1993. He was engaged most recently in small-angle scattering measurements on supported-metal catalysts using Synchrotron Radiation. He was a visiting scholar at the U. of Graz (Austria), the Weizmann Inst. of Science (Israel), the U. of Cambridge (England), and the Swiss Federal Inst. of Technology (ETH) (Zürich, Switzerland). His publications are characterized by concision and clarity. The same desire for clarity informed his teaching. His adeptness at puncturing pomposity and signaling unclear thinking in others probably did not endear him to everyone. Receiving correspondence from Harry was a great pleasure, due equally to the elegance of the writing style and the intelligence of the content. In an interview Harry told a reporter about the joys of scientific research, and how they made all the hardships worthwhile. His devotion to his research is one of the things we will long remember. We will also miss his elegance, wit, erudition, and the other qualities which made him such a great colleague and friend.

J. Goodisman, USA, S. Ciccariello, Italy, G. Kostorz, Switzerland